LINEAR–RESPONSE PROGRAM PACKAGE "LMTO MAGNONS"
USER's MANUAL

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1 INTRODUCTION

The linear–response linear-muffin-tin-orbital (LR-LMTO) programs described here are designed to perform linear–response calculations of the dynamical spin and charge susceptibilities for arbitrary wave vectors $\mathbf{q}+\mathbf{G}$ and frequency ω within the methods of time–dependent density functional theory (TD–DFT) (Refs. [1, 2, 3, 4]).

The development described here is analogous to the linear–response calculation of the lattice dynamics and electron–phonon interactions which has been described in several publications [5, 6, 7, 8]. A short description of the method for calculating dynamical susceptibilities is appeared recently [9].

The purpose of the linear–response method is to find change in charge density and magnetization induced by a perturbation of a ceratin wave vector $\mathbf{q}$. If one is interesting by the dynamical spin or charge susceptibility $\chi(r,r',\omega)$, the perturbation is given by either scalar external potential $\delta V_{ext}(r,t) = \delta v \exp[i(\mathbf{q}+\mathbf{G})\mathbf{r}+\omega t]$ or external magnetic field.$\delta B_{ext}(r,t) = \delta b \exp[i(\mathbf{q}+\mathbf{G})\mathbf{r}+\omega t]$ Fixing wave vector $\mathbf{q}$, selecting reciprocal lattice vector $\mathbf{G}$ and the frequency ω the problem is reduced to the self–consistent solution of a differential equation (so–called Sternheimer's equation) which is a linearized version of Schrödinger's equation. Solving this problem self–consistently gives an access to the function $\chi(\mathbf{r},\mathbf{q}+\mathbf{G},\omega)$ which is the susceptibility Fourier transformed over one index. The entire problem is very similar to the self–consistency problem of standard band–structure calculation. It is however much more heavy to solve it numerically because finding $\chi(\mathbf{r},\mathbf{q}+\mathbf{G},\omega)$ for a grid of wave vectors $\mathbf{q}+\mathbf{G}$ requires N_{q+G} (total number of $\mathbf{q}+\mathbf{G}$ points) self-consistent calculations performed for a set of frequencies ω. It therefore requires $N_{q+G} \times N_\omega$ self–consistent calculations, each of them being equivalent to the standard band structure calculation for the *unperturbed* system.

Linear–response calculations of $\chi(\mathbf{r},\mathbf{q}+\mathbf{G},\omega)$ should, in principle, not be so sensitive to the details of the charge density distribution over the cell. However a full–potential (FP) solution of the problem is desired. According to different treatment of the full–potential terms in the band structure calculations performed with the original FP-LMTO method (for the description of these programs see FULL-POTENTIAL LMTO PROGRAMS "NMT": USER's MANUAL, which is available on the WEB site under the address: http://www.mpi-stuttgart.mpg.de/docs/ANDERSEN/) there are two linear–response programs: MAGASA and MAGPLW. MAGASA uses atomic sphere approximation and does not treat interstitial region correctly. MAGPLW uses plane–wave representation for all the relevant quantities in the interstitial region, and, therefore, much more accurate. Note that MAGPLW code is much slower than MAGASA program.

The purpose of these MAG* programs is to calculate $\chi(\mathbf{r},\mathbf{q}+\mathbf{G},\omega)$ The basic input to the program is given by the charge density distribution of the unperturbed crystal. It is therefore necessary to install and learn how to use the programs NMTASA and/or NMTPLW for the original self–consistent band structure calculations with the LMTO method, This program uses the same plane–wave representation for the charge densities and the potentials in the interstitial region. (The package of programs NMT including three versions NMTASA,NMTCEL and NMTPLW is distributed separately and can be downloaded from http://www.mpi-stuttgart.mpg.de/docs/ANDERSEN/SAVRASOV/frames.htm)

Finding $\chi(\mathbf{r},\mathbf{q}+\mathbf{G},\omega)$ is divided in two parts which run independently:

- *Preparational part*: A self–consistent band structure calculation with the NMTASA or NMTPLW code must be performed for the original crystal. A self–consistent charge density file (SCFFILE) must be created.

- *Self–consistency part*: Self–consistent linear–response calculation is performed for each wave

vector $\mathbf{q}+\mathbf{G}$, frequency ω and for either external scalar potential field (for finding charge susceptibility) or for external magnetic field (for finding spin susceptibility) using the package MAGASA or MAGPLW. For magnetic field calculation, there is additional parameter μ=-1,0,1 fixing polarization of the field in spherical coordinates. The main input file to the NMT* program INIFILE is used as the main input control file in the MAG*. Also, a list of wave vectors $\mathbf{q}+\mathbf{G}$ must be prepared before running MAG* and stored in the file (called PNTFILE). Another input control file (called LRTFILE) must be prepared (typical example will be given). The change in charge density for each $\mathbf{q}+\mathbf{G}, \omega, \mu$ will be calculated by MAG* and stored in two kinds of files referred as DROFILE and DPSFILE. DROFILE contains change in charge density expanded in spherical harmonics within MT–spheres and DPSFILE contains change in charge density expanded in plane waves in the interstitial region. There is as many DROFILEs and DPSFILEs as $3 \times N_q \times N_{atom}$.

All programs described in this manual can be downloaded from http://www.mpi-stuttgart.mpg.de/docs/A
About the notations in this document:

- all file names like **nbc.ini, main.exe**, are boldfaced.
- all directory names like */magplw/dat/* are italicized.
- capitalized names like INIFILE, STRFILE are made to shorten references to the MAIN INPUT CONTROL FILE (for INIFILE), STRUCTURE CONTROL FILE (for STRFILE), etc.

I apologize if the description of some parameters is short and unclear. Any suggestions to improve this manual are welcomed. I also cannot guarantee that all the bugs in the programs are found. Since linear–response calculation is a relatively new field in computational solid–state physics there could be some other problems, instabilities in the algorithms which have been used in the programs. Any further improvements of the programs are welcomed.

2 INSTALLATION

In this section the directories which are used for running the programs and storing input/output data are described. The MAG* packages have the directory organization similar to the packages NMT*. There exists three main directories:

- */magasa/ /magplw/*- directories containing source code of the main LR-LMTO programs MAGASA/MAGPLW designed to perform self–consistent linear–response calculations. Input data files and some auxiliary programs are also stored in this directory.
- */maglib/* - directory containing a number of other application programs helping to construct input data and understand output information.

Below the contents of each of the directories is described. The */magasa/* and */magplw/* have two subdirectories:

- */magasa/run/,/magplw/run* - directories containing the source code ***.f** of the main LR-LMTO programs MAGASA,MAGPLW (text of the program written on FORTRAN77), object files ***.o** and executable file usually named as **main.exe**.
- */magasa/dat/,/magplw/dat/* - directories with the input/output data files to the main LR-LMTO program. Usually, many subdirectories are created here according to the element (compound) name to be calculated. An example of the compound which will be considered below is ferromagnetic iron. The input/output data files are contained in */magplw/dat/fe/* directory.

There exists a library directory */maglib/*. It containes a number of auxiliary programs. The programs understand input/output data files of the MAG* codes. The contents of */maglib/* is

- */maglib/qpnt/* - program which generates irreducible set of **q**-points according to the input divisions and stores them into the PNTFILE. The latter is one of the input files to the MAG* codes. Note that the perturbation wave vectors **q** must be chosen to have minimal length (one of the options while running QPNT) in order to have well–convergent plane–wave expansions (see below).

All programs and data files are tared and gzipped into 2 files named as **magasa.tar.gz, magplw.tar.gz,** and **maglib.tar.gz**

1. **gunzip magasa.tar.gz**
2. **tar -x -f magasa.tar**

Repeat these steps for **magplw.dec**, and **maglib.dec**.

3 RUNNING MAGASA/MAGPLW PROGRAMS

In this section general hints how to run main linear-response codes MAGASA/MAGPLW are described. Section USING MAGLIB LIBRARY will describe how to run auxiliary library routines.

3.1 Configuring MAGASA/MAGPLW

To be able to run MAGASA/MAGPLW it is necessary to compile the source data files. A few comments must be said here. First, the maximum size of every array (such as maximum number of atoms, l_{max}, etc) in the program is declared using the Fortran PARAMETER statement. These statements are contained in the file PARAM.DAT. (See Section PARAMETER FILE: PARAM.DAT for the detailed description) The file PARAM.DAT is included into every source code during the compilation time by INCLUDE statement. The second comment concerns a scratch file storage. To minimize core memory, some data during the run are temporary stored in the scratch files. To be able to do this, a scratch directory must exist on any particular node where execution of the program is performed.

To create executable file of the MAG* program, go to the directory */mag*/run/*.

1. Edit PARAM.DAT and install the necessary size of arrays. Sample PARAM.DAT file is provided.
2. Edit the file **setup.f** and specify the path to the scratch directory. Also check that other set-up data match with your local operational system.
3. Edit the file **timel.f** and specify the call to the system subroutine to learn CPU time.
4. Compile all programs, link them to get executable file **main.exe**. Under UNIX, using AIX XL Fortran Compiler this looks like: **xlf -cOw *.f** to compile only, with optimization, and suppressing all warning messages. The command **xlf -cCg *.f** will compile only, suppress optimization and provide debugging information. To link, use the command **xlf *.o -o main.exe**. To create a load map use the command **xlf *.o -o main.exe -bloadmap:map**. At the end of the map file a total amount of the core memory allocated by the program is printed out.

To run MAG* for a particular compound, create a subdirectory in */mag*/dat/*. For example, to calculate χ of Fe, create */magplw/dat/fe/*. In this subdirectory, create the following subdirectories (this is default list of the subdirectories listed in the linear-response control file LRTFILE. See also chapter LINEAR RESPONSE CONTROL FILE: LRTFILE.)

- */magplw/dat/fe/INP/* subdirectory for storing input files, like main input control file INIFILE, structure control file STRFILE, self–consistent charge density file SCFFILE, linear response control file LRTFILE, etc.
- */magplw/dat/fe/DRO/* subdirectory for storing the files with changes in charge density and pseudodensity. All names for these files will be given automatically.
- */magplw/dat/fe/WGT/* subdirectory for storing the files containing the **k** space integration weights. All names for these files will be given automatically.

Note that the directory INP contains the files which are unique for all $\mathbf{q} + \mathbf{G}$ points and frequencies ω. All other directories contain the files which are specific for any particular **q+G** point, ω and field polarization. Since there are too many files ($4 \times N_{q+G} \times N_{\omega}$) their filenames are constructed automatically. For example, the rule to construct the name for DROFILE is (i) three first letters are **dro**, (ii) **q**–point number, (iii), G-vector number, (iv) ω, (v) polarization. Polarization μ=-1 abbreviated as "m", μ=0 abbreviated as "z", and μ=+1 abbreviated as "p". If scalar potential

field is used for charge susceptibility, it is abbreviated as "v". For example, when one finds self-consistent response for the **q**–point number 12 (listed in PNTFILE), G-vector 3, $\omega = 30$ meV, and polarization z along magnetization axis, the change in charge density (DROFILE) will be stored in the file **dro12g03w30z** and will be automatically placed into the directory *DRO*. Analogously names are constructed for DPSFILEs, etc.

3.2 Terminal input

MAGASA/MAGPLW programs have several input lines:

IFOLDER?
INIFILE?
SCFFILE?
STRFILE?
LRTFILE?
Q-POINT?
G–SHELL?
FREQUEN?
RUNMODE?
RUNTASK?

The answers must be either given from the terminal or placed into a job file. General description of the input lines is given below:

- IFOLDER gives the subdirectory name where all input files are stored. For example, if the input subdirectory is called INP/, the string "INP/" must be given to the answer "IFOLDER?".
- INIFILE is a name of the main control data file. The structure of the file is identical to the INIFILE of the NMT package. A description of this file and its difference to that of the NMT package will be given in section MAIN CONTROL FILE: INIFILE. INIFILE must be stored in the subdirectory specified by the parameter IFOLDER.
- SCFFILE is a name of the self-consistent charge density file which is calculated by the NMTASA/PLW packages. SCFFILE must be stored in the subdirectory specified by the parameter IFOLDER.
- STRFILE is a name of the structure data file. It is the same as used by the NMT* package, therefore it is not described in this manual. STRFILE must be stored in the subdirectory specified by the parameter IFOLDER.
- LRTFILE is a name of the linear-response control file. This file is specific for linear response calculation and does not contain any information about the compound. Its detailed description will be given below in the section LINEAR RESPONSE CONTROL FILE: LRTFILE. LRTFILE must be stored in the subdirectory specified by the parameter IFOLDER.
- Q-POINT is a **q**–point number. A list of **q** points must be prepared and stored in the PNTFILE. Use program QPNT located in */maglib/qpnt/* for this purpose. (See section USING MAGLIB LIBRARY for the detailed description). Lines in the PNTFILE numerate **q** points. A path to the PNTFILE is contained in the INIFILE. Therefore setting Q-POINT number from the terminal will result in reading the corresponding line from the PNTFILE. Note that Q-POINT

number must be set as a *character* string. The reason is that all output files containing change in charge densities, potentials, etc, must be named differently for different **q** points. The character string specifying **q** point will be added to any output filename. For example,

Q-POINT? 01

means that the first point from PNTFILE will be treated as a perturbation wave vector and the string **01** will be added to any of the output files.

- G-SHELL shows which of the reciprocal lattice vectors will be added to q–point in order to make a perturbation vector $\mathbf{q}+\mathbf{G}$. Reciprocal lattice vectors are generated by shells in the reciprocal space and stored in the PNTFILE. G-SHELL=0 corresponds to G=0, then follows first, second, etc. shells. Setting G–SHELL equal to 1 will consider a given q–point plus all reciprocal lattice vectors G which belong to a given shell as perturbation vectors q+G. Some of these vectors can be connected by symmetry operations. Note that $\mathbf{G}\neq 0$ are only necessary to apply external fields changing within the unit cell. All acoustic magnon modes, for example, are seen by considering only **q** with **G**=0. To find optical magnon modes, it is necessary to apply non–zero **G.**

- FREQUEN gives the frequency in meV. Note that FREQUEN must be set as a *character* string. The reason is that all output files containing change in charge densities, potentials, etc, must be named differently for different ω The character string specifying ω will be added to any output filename. For example,

  FREQUEN? 0300

  means that $\omega = 300$ meV will be treated as the perturbation frequncy and the string **0300** will be added to any of the output files.

- RUNMODE shows in which mode the program will be executed. The following answers can be given:

  - 0 : preparational mode. Only the bands for a large number of k-points will be calculated. Use this mode when calculating metals. For correct treatment of the effects of the Fermi surface, the knowledge of the energy bands at a dense grid is required. This mode will prepare the necessary file.
  - 1 : starting self–consistency mode. Use this mode when nothing is done with the self–consistency for a given **q** point. That means that the change in charge density is not known (no DROFILE and DPSFILE exist)
  - 2 : continuation of the self–consistency. Use this mode when self–consistency for a given **q** point is continuing with the same set up (# of **k** points and other data were not changed). DROFILE and DPSFILE must exist at this step, but by some reason self–consistency is not finished. Actually, if one sets RUNMODE=2 and the program will not find corresponding DROFILE and DPSFILE, the mode will be automatically set to one.

- RUNTASK selects polarizations: *m,z,p* stand for applied magnetic fields polarized along -1,0,1 axis. Note that the magnetization axis is always given by z–axis. Therefore in order to study transverse spin fluctuations in ferromagnets, only m and p polarizations should be considered. Another keyword *v* stands for applied scalar external potential in order to study charge response.

4 MAIN CONTROL FILE: INIFILE

The main control file of the linear-response package is very similar to that of the NMTASA/PLW packages. It has an extension **.ini**. Below an example of magnon spectrum calculation for Fe is considered. The INIFILE for Fe has the name **fe.ini** or more shortly **ini**. It can be created easily from the INIFILE of the NMT package. Only a few lines must be edited there. Let's consider this example:

```
*** Band Structure Calculation of bcc-Fe ***
-----------------------------------------------------------------
Control Parameters :
 3                              - lift
 1                              - lmto
 0                              - nsph
 1                              - lrwf
 0                              - npfr
Exchange-Correlation Code :
 14                             - 1,2,3 :by VBarth-H;Gunn-L;Jan-W
Iterative Procedure Limits and Accuracy :
 50,0.2,0.2,1.D-4,+6 0,0.3,0.3  - niter,mix,mag,eps,lbr,ibr,mixb,mixh
Atomic Data :
 1,1,2,1                        - natom,nsort,nspin,norbs
 5.425,1.0                      - lattice parameter,v/v0
 1                              - is(iatom)
 3 (-0.05,0.0),(-1.0,0.0),(-2.5,0.0) - Nkap, Ekap(ikap)
for Fe                          ----------------------
 26.D0 18.D0,1,1,0,0.5D0,55.847 - z zcor,lr,icor,ispl,split,mass
 2.349,1.D0,1.D0,0.D0           - mt-sphere,rou-sphere,weight,rloc
 6 2 6                          - lmax-t,lmax-b,lmax-v
valence states are :
 s p d f                        - states for E=0.5 Ry
 4 4 3 4                        - main quantum numbers
 1 1 1 0                        - basis set
 3 3 3 0                        - choice of Eny
 0.30, 0.30, 0.30, 0.50         - Eny
 0.30, 1.60,-1.50,-3.00         - Dny
 s p d f                        - states for E=0.5 Ry
 4 4 3 4                        - main quantum numbers
 1 1 1 0                        - basis set
 3 3 3 0                        - choice of Eny
 0.30, 0.30, 0.30, 0.50         - Eny
 0.30, 1.60,-1.50,-3.00         - Dny
 s p d f                        - states for E=0.5 Ry
 4 4 3 4                        - main quantum numbers
 1 1 1 0                        - basis set
 3 3 3 0                        - choice of Eny
 0.30, 0.30, 0.30, 0.50         - Eny
```

```
 0.30, 1.60,-1.50,-3.00         - Dny
semicore states are :
 0                              - # of states
Input Control Files :     ------------------------
 2 'fe.con'                     - icon,<confile>
 0 'fe.tmp'                     - itmp,<tmpfile>
 2 'fe.psi'                     - ipsi,<psifile>
 0 'fe.tmp'                     - itmp,<tmpfile>
 2 'fe.bnd'                     - ibnd,<bndfile>
 0 'fe.pot'                     - ipot,<potfile>
 0 'fe.ptn'                     - iptn,<ptnfile>
 0 'fe.dos'                     - idos,<dosfile>
 2 'fe.scf'                     - iscf,<scffile>
 2    'out'                     - iout,<outfile>
Other Data for Mag-Pack :
 0,9,0.1                        - nff,nef,de
 16,16,16,32                    - n1,n2,n3,nc
 20,20,20,0.02,0.04,0,10        - nfft1,nfft2,nfft3,epsr,epsg,kbz,bzr
Additional input files:
 0 'fe.hub'                     - ihub,<hubfile>
 0 'fe.hop'                     - ihop,<hopfile>
 0 'fe.opt'                     - iopt,<optfile>
 2 'fe.enr'                     - ienr,<enrfile>
 2 'fe.pnt'                     - ipnt,<pntfile>
```

This file is unique and is used to perform self–consistent calculations for all $\mathbf{q}$,$\mathbf{G}$,ω, μ. Only a few lines are treated differently from the input to NMTASA/PLW programs. It will be explained below:

4.1 Control Parameters

```
*** Band Structure Calculation of bcc-Fe ***
-----------------------------------------------------------------
Control Parameters :
 3                              - lift
 1                              - lmto
 0                              - nsph
 1                              - lrwf
 0                              - npfr
```

This set of parameters should be exactly the same as used in the NMTASA/PLW calculation. Note that the keyword *lrwf* should be set to 1 when preparing the SCFFILE by NMTASA/PLW.

4.2 Exchange-correlation functional

```
Exchange-Correlation Code :
 14                             - 1,2,3 :by VBarth-H;Gunn-L;Jan-W
...
```

The exchange–correlation should be the same as used in the NMTASA/PLW calculation.

4.3 Iterative Procedures Limits and Accuracies

```
Iterative Procedure Limits and Accuracy :
 50,0.2,0.2,1.D-4,+6 0,0.3,0.3  - niter,mix,mag,eps,lbr,ibr,mixb,mixh
```

This set of parameters has the same meaning as in the NMTASA/PLW calculation, but they are used for calculating *changes* in charge density. The meaning of every parameter is given below:

- *niter*: max. number of iterations for doing self-consistency of the change in charge density for given $\mathbf{q}$,$\mathbf{G}$,$\omega\mu$.
- *mix*: starting mixing of the charge density in linear mixing scheme. During the iterations towards self–consistency the mixing will be optimally adjusted according to the Pratt scheme. This parameter is ignored if Broyden mixing (see below) is switched on.
- *mag*: starting mixing for the magnetization in linear mixing scheme. During the iterations towards self-consistency the magnetization mixing will remain constant and will NOT be adjusted. The parameter has no effect for non–spin–polarized calculations or if Broyden mixing (see below) is switched on.
- *eps*: charge density convergency criterion. Typically 10^{-2}. The program will stop doing self–consistency for a particular $\mathbf{q}$,$\mathbf{G}$,$\omega\mu$.if the mean square difference between two induced densities in consequent iterations is less then *eps*. Note that if a few displacements and polarizations run spontaneously, the program will automatically terminate iterating those displacements which reach self–consistency. Also note that the reached convergency is written to the DROFILE. When restarting the execution, the program will check whether for a given displacement and polarization reached accuracy is higher than input *eps* or not. If it is higher, number of iterations for this displacement and polarization will be automatically set to 0, if it is not, then the iterational cycle will continue. You can also use this when it is necessary to improve convergency of the induced charge density. Suppose it is self–consistent with the accuracy, say, 10^{-2}. In order to improve the convergency, reset *eps* from 10^{-2} to, say, 10^{-4} in the INIFILE. The iterational cycle for given displacement and polarization will be renewed.
- *lbr*: switches on the Broyden mixing. If -1 then Broyden is OFF, if 0 then Broyden is ON for l=0 component of $\delta\rho(\mathbf{r})$, if +1,+2 then Broyden is on for *l*.le.*lbr* component of Drho(r). It is highly recommended to set lbr to the $\mathrm{l_{max}}$ value of spherical harmonics expansions for the charge density and potential. It is controlled by the parameter LmaxV (see below) and it is usually 4 (for ASA) or 6 (for PLW). Broyden restarts every time after NTERMAX iterations. Parameter NTERMAX is in PARAM.DAT. Usually NTERMAX=15.
- *ibr* starts Broyden after I=*ibr* iterations. If *ibr*=0 then start immediately. If *ibr*>0 then first I=*ibr* iterations will be done with the linear mixing scheme where the mixing parameters *mix* and *mag* are specified above.
- *mixb*: this is initial guess for Jacobian which is closely related to mixing parameter *mix* in the linear mixing scheme. It was found that *mixb* cannot be small and it is usually of the order 0.3-0.4

- *mixh*: this is linear mixing parameter for higher l-components (l>lbr) of the charge density. Since it is assumed that these components do not influence much the self-consistence loop, they are mixed within linear mixing scheme and do not stored for all previous iterations.

4.4 Atomic Data

```
Atomic Data :
 1,1,2,1                          - natom,nsort,nspin,norbs
 5.425,1.0                        - lattice parameter,v/v0
 1                                - is(iatom)
 3 (-0.05,0.0),(-1.0,0.0),(-2.5,0.0) - Nkap, Ekap(ikap)
```

This set of parameters should be exactly the same as used in the NMTASA/PLW calculations. Note that an option switching spin-orbit coupling is not yet available for the linear–response magnon program. Note also that *number of spins must ALWAYS be set to 2 when using MAGASA/PLW.*

```
for Fe                           ----------------------
 26.D0 18.D0,1,1,0,0.5D0,55.847 - z zcor,lr,icor,ispl,split,mass
 2.349,1.D0,1.D0,0.D0            - mt-sphere,rou-sphere,weight,rloc
 6 2 6                           - lmax-t,lmax-b,lmax-v
```

This set of parameters should be the same as used in the NMTASA/PLW calculation.

- *for Nb*: title for every atom. Note that this character string (maximum 10 letters) will be read and widely used in the output file. Therefore it is recommended to use the format "for EL"
- *z*: atomic number.
- *zcor*: deep-core charge.
- *lr*:
  - 0 for non-relativistic calculations,
  - 1 for scalar-relativistic valence states
- *icor*: this parameter has no effect for linear–response calculation.
- *ispl,split*: both these parameters have no effect for linear–response calculation.
- *mass*: atomic mass of the element as in the periodic table.
- *mt-sphere*: non-touching muffin-tin sphere radius.
- *rou-sphere*: this parameter has no effect for linear–response calculation using MAGASA/PLW packages.
- *weight*: this parameter has no effect for linear–response calculation.
- rloc: this parameter has no effect for linear–response calculation.

- *lmax-t*: maximal angular momentum l (not $l+1$!) for the basis functions (i.e. for the decomposition of the tails coming from other atoms). Normally it is 6 for PLW calculation.
- *lmax-b*: maximal l actually included in basis.
- *lmax-v*: maximal l-value for the expansion of the induced charge density and the induced potential in spherical harmonics. Normally it is the same as *lmax-t*.

The following block is repeated for each κ from 1 to *nkap*:

```
valence states are :
 s p d f                        - states for E=0.5 Ry
 4 4 3 4                        - main quantum numbers
 1 1 1 0                        - basis set
 3 3 3 0                        - choice of Eny
 0.30, 0.30, 0.30, 0.50         - Eny
 0.30, 1.60,-1.50,-3.00         - Dny
 s p d f                        - states for E=0.5 Ry
 4 4 3 4                        - main quantum numbers
 1 1 1 0                        - basis set
 3 3 3 0                        - choice of Eny
 0.30, 0.30, 0.30, 0.50         - Eny
 0.30, 1.60,-1.50,-3.00         - Dny
 s p d f                        - states for E=0.5 Ry
 4 4 3 4                        - main quantum numbers
 1 1 1 0                        - basis set
 3 3 3 0                        - choice of Eny
 0.30, 0.30, 0.30, 0.50         - Eny
 0.30, 1.60,-1.50,-3.00         - Dny
```

The meaning of these parameters is exactly the same as in the INIFILE of the NMT package.

4.5 Input Control Files:

```
Input Control Files :     -----------------------
 2 'fe.con'                     - icon,<confile>
 0 'fe.tmp'                     - itmp,<tmpfile>
 2 'fe.psi'                     - ipsi,<psifile>
 0 'fe.tmp'                     - itmp,<tmpfile>
 2 'fe.bnd'                     - ibnd,<bndfile>
 0 'fe.pot'                     - ipot,<potfile>
 0 'fe.ptn'                     - iptn,<ptnfile>
 0 'fe.dos'                     - idos,<dosfile>
 2 'fe.scf'                     - iscf,<scffile>
 2    'out'                     - iout,<outfile>
```

This section gives the names of the files which are used by the program. The consequence of the files is the same as in the INIFILE of the NMT* programs. The meaning of the control parameters is the following:

- 0 - file is not created, or created as temporary.
- 1 - file will be opened as a new one and saved, if file exists, the execution will be terminated.
- 2 - file already exists and will be read, if file does not exist, the switch will be automatically set to 1.
- 6 - the contents of the file will be printed out to the terminal. (channel #6)
- *icon,<confile>*: this is the structure constants file which will be created by MAGASA/PLW at the beginning. Note that the CONFILE created by MAGASA/PLW cannot be used by the program MAGASA/PLW. Keep structure constants in the INP directory to make them shareable when running different **q** points spontaneously. Always set *icon*=2.
- *itmp,<tmpfile>*: this parameter is not used by MAGASA/PLW.
- *ipsi,<psifile>*: this is the file which contains wave functions on the grid of **k** points in the IBZ. Keep wave functions in the INP directory to make them shareable when running different **q** points spontaneously. Always set *ipsi*=2.
- *iscr,<scrfile>*: this is the first character string for the scratch file names. Scratch files will be created in the temporary directory. The path to the temporary directory is contained in the file */mag*/run/***setup.f**. Always set *iscr*=0.
- *ibnd,<bndfile>*: this is the file which contains energy bands on the grid of **k** points in the IBZ. Keep energy bands in the INP directory to make them shareable when running different **q** points spontaneously. Always set *ibnd*=2.
- *ipot,<potfile>*: this file is not used by MAGASA/PLW.
- *ifat,<fatfile>*: this file is not used by MAGASA/PLW.
- *idos,<dosfile>*: this file is not used by MAGASA/PLW.
- *iscf,<scffile>*: this file is not used by MAGASA/PLW. Name for the SCFFILE which contains the self-consistent charge density distribution for the original crystal as calculated by the program NMTASA/PLW, will be read from the terminal. SCFFILE must be prepared before running linear–response code! For convenience, place it into the INP directory.
- *iout,<outfile>*: this is the current output file in this run. In fact, it is first character string of the filename. The final name will also contain **q**–point number as it was read from the Q-POINT input line, frequency name as read from FREQUEN input line, and also task name, as it was read from the RUNTASK input line. Set *iout*=2 if storage is necessary, set *iout*=6 to print the current output to the terminal. Note that this file will be created NOT in the INP directory as it is done with CONFILE,BNDFILE, and PSIFILE, but in the root directory.

4.6 Other Data for MAG-pack

```
Other Data for Mag-Pack :
 0,9,0.1                          - nff,nef,de
 16,16,16,32                      - n1,n2,n3,nc
 20,20,20,0.02,0.04,0,10          - nfft1,nfft2,nfft3,epsr,epsg,kbz,bzr
```

This set of parameters is similar to what is used in the NMTPLW calculation. However there are differences. The exact meaning is given below:

- *nff,nef* : number of filled bands in the main valence panel (above the semicore!) and number of bands crossing the Fermi level. These parameters must be chosen with more care in contrast to NMTPLW, see subsection "Notes to k-space integration" for the detailed description.
- *pole:* parameter connected with the Lorentizan broadening of the Fermi surface integrals. The parameter is not used by NMTPLW. See also subsection "Notes to k-space integration".
- *nk1, nk2, nk3*: divisions of the Brillouin zone along three directions for the tetrahedron integration. (see subsection "Notes to k-space integration").
- *nw1*: divisions of the Brillouin zone along three directions for finding the weights in the tetrahedron integration. Only the first division must be specified, two others *nw2, nw3* will be calculated according to nk1, nk2, nk3. Note that this parameter substitutes the parameter *nc* of the NMTPLW. See subsection "Notes to k-space integration" for the detailed description.
- *m1, m2, m3:* divisions of the unit cell for the fast Fourier transform. These parameters should be the same as used by the NMTPLW calculation.
- *epsR, epsG* : accuracy of matching the spherical Hankel functions in real and reciprocal space. These parameters should be the same as used by the NMTPLW calculation.
- *keyt, bzr:* to accelerate Fourier transforms when calculating interstitial potential matrix elements, set *keyt*=1. In this case the radius of the cutoff sphere in reciprocal space is set by parameter *bzr* times the radius of the sphere circumscribing the Brillouin zone. Usually it is 4-6. The smaller *bzr* value the faster calculation the lower the accuracy. These parameters should be the same as used by the NMTPLW calculation.

Finally, path to additional input files must be specified

```
Additional input files:
 0 'fe.hub'                       - ihub,<hubfile>
 0 'fe.hop'                       - ihop,<hopfile>
 0 'fe.opt'                       - iopt,<optfile>
 2 'fe.enr'                       - ienr,<enrfile>
 2 'fe.pnt'                       - ipnt,<pntfile>
```

- ihub,<hubfile>: this parameter has no effect in the linear-response calcualtion.
- ihop,<hopfile>: this parameter has no effect in the linear-response calcualtion.

- iopt,<optfile>: this parameter has no effect in the linear-response calcualtion.

- *ipnt,<pntfile>*: this is the file which contains a list of the wavevectors **q** for linear–response calculations (so called PNTFILE). Use program QPNT located in */maglib/qpnt/* to prepare PNTFILE. (See section USING MAGLIB LIBRARY for the detailed description). Lines in the PNTFILE numerate **q** points. Therefore setting Q-POINT number from the terminal will result in reading the corresponding line from the PNTFILE. For convenience, place it into the INP directory. Always set *ipnt*=2.

- *ienr,<enrfile>*: this is the file which contains energy bands on the dense grid of **k** points in the IBZ (see subsection "Notes to k-space integration"). Keep energy bands in the INP directory to make them shareable when running different **q** points spontaneously. Always set *ienr*=2.

4.7 Notes to k-space integration

This section explains how to handle with the parameters responsible for the **k**–space integration which is performed to find change in charge density for every vector **q**. This set of parameters involves *nff, nef* - number of bands below and crossing the Fermi level, *pole* - Lorentzian broadening, *nk1,nk2,nk3* - BZ divisions for integration, *nw1,nw2,nw3* - BZ divisions to find the integration weights, and *<enrfile>* - file which contains energy bands generated at the grid set up by *nw1,nw2,nw3*.

For semiconductors, when there is an energy gap between occupied and unoccupied states, the **k**–space integration using misweight–free tetrahedron method is equivalent to the special point method. In this case set *nff* to the actual number of bands below the Fermi energy, *nef* to zero, *pole* to zero, specify the grid parameters *nw1,nw2,nw3* equal to the BZ divisions *nk1,nk2,nk3*. ENRFILE which contains the bands generated at the grid *nw1,nw2,nw3* will be the same as the BNDFILE which contains the bands generated at the grid *nk1,nk2,nk3*. These files will be created automatically after one run of the main program.

For metals, it is possible (without lost of computer time) to essentially improve accuracy of the BZ integration using multigrid technique. The idea is based on the fact that the effects of energy bands and of the Fermi surface can be taken into account exactly in the linear–response calculation. While matrix elements necessary to construct induced charge density are calculated at the coarse grid (set up by the numbers *nk1,nk2,nk3*), the weights for the **k**–space integration which take into account the exact shape of the Fermi surface can be found using the bands generated at the dense grid (set up by the numbers *nw1,nw2,nw3*). Two grids must commensurate with each other. To reach this purpose, first ENRFILE which contains the bands at the dense grid must be created. To create ENRFILE, just specify RUNMODE=0. The program will automatically generate **k** points according to *nw1,nw2,nw3*, will do only one band calculation, will store ENRFILE and will stop. Using any RUNMODE different from 0 will pick up coarse **k**–space grid according to *nk1,nk2,nk3*. During the construction of the weights for the integration, information stored in the ENRFILE will be taken into account.

In order to choose numbers of bands below and crossing the Fermi level, use the following hint. Look at the bands in the Γ point. (They usually printed out in the OUTFILE). Locate the band nearest to the Fermi energy. Step out from this band by approximately 0.5 Ry down. Count the bands below this energy, they can be treated as filled bands *nff*. The bands located at the energy window plus/minus 0.5 Ry from the Fermi energy should be treated as the bands crossing E_F (*nef*). Set lorentizan broadening parameter *pole* to approximately 0.1 Ry.

Note that any wave vector **q** must belong to the grid generated by *nk1,nk2,nk3* and *nw1,nw2,nw3*. In other words, grid of wave vectors **q** set-up by three numbers *nq1,nq2,nq3* (see section USING MAGLIB LIBRARY) must commensurate with the grids *nk1,nk2,nk3* and *nw1,nw2,nw3*. Normally, select such *nq1,nq2,nq3* when the number of irreducible **q** points generated is not more than 20-40. The grid for **k**–space integration can be the same (*nk1,nk2,nk3=nq1,nq2,nq3*) or not more than twice denser. Do not use very many **k** points here, all **k**–space integrals are fastly convergent. The grid *nw1,nw2,nw3* is the same as the grid *nk1,nk2,nk3* for semiconductors. For metals, use *nw1,nw2,nw3* which is 3-5 times denser than the grid *nk1,nk2,nk3*. The number of irreducible **k** points for integration weights should be of the order 1000.

Final note must be said when calculating electron–phonon matrices (RUNMODE=5). Since the corresponding BZ–integrals are very sensitive to the divisions *nk1,nk2,nk3* use the following hints. (i) Reach self–consistency for all **q**–points, all displacements and all polarizations. All DROFILEs and DPSFILEs must be created and stored in the DRO directory. (Calculate dynamical matrix and the phonon spectrum for every q–point when for this q–point self–consistency is reached for all displacements and all polarizations). (ii) Delete contents of the directory WGT which contains the weights for the BZ integration. (iii) Make a new INIFILE in which specify the divisions *nk1,nk2,nk3* of the coarse grid equal to the divisions *nw1,nw2,nw3* of the dense grid, the number of irreducible **k** points for integration must be of the order 1000. Carefully set the number of bands below/crossing the Fermi level equal to the actual number of bands below/crossing the Fermi level. Delete or rename BNDFILE and CONFILE since they contains the information generated for the coarse grid. (iv) Run the main program with the RUNMODE=5. CONFILE and BNDFILE will be created. Also a new PSIFILE with the wave functions will be created. However, the wave functions will be stored only for the bands crossing the Fermi level (that's why it is necessary to reset this number, otherwise this file will have a huge size!). (v) After CONFILE, BNDFILE, and PSIFILE are created at the dense grid *nk1,nk2,nk3=nw1,nw2,nw3*, run different **q** points to calculate the electron–phonon matrices. The new weight files will be created automatically and stored in the *WGT* directory. Note that the integration weights for the electron–phonon matrices are different from those which have been using to find the induced charge densities, that's why it is necessary to delete the contents of the directory *WGT* before using RUNMODE=5. The calculation of the electron–phonon matrix is computationally much more faster than making self–consistency and finding dynamical matrix.

5 LINEAR–RESPONSE CONTROL FILE: LRTFILE

LRTFILE is used to set up the data which are specific for linear response calculations. In fact, this file does not contain an information on the compound to be calculated and, therefore, the LRTFILE does not have to be modified except some special cases. A typical LRTFILE is given below:

```
SET-UP DATA FOR LINEAR RESPONSE CALCULATIONS
----------------------------------------------------
GENERAL SETTINGS:
'Magnons   '                  - Response scheme (Phonons/Magnons)
'Plz=off'                     - Polarizabilty on/off
'Stn=off   '                  - Stoner renormalization on/off
'Del=on    '                  - Changes in radial functions on/off
'Dyn=none  '                  - Dynamical matrix scheme (none,hf,oka1,oka*)
DEFAULT FILE SETTINGS:
 0 'DSF/dsf'                   - idsf,<dsffile>
 2 'WGT/wgt'                   - iwgt,<wgtfile>
 0 'TMP/tmp'                   - itmp,<tmpfile>
 0 'STN/stn'                   - istn,<stnfile>
 0 'PHN/phn'                   - iphn,<stnfile>
 0 'PLZ/plz'                   - iplz,<plzfile>
 0 'PLZ/pls'                   - ipls,<plsfile>
 0 'POT/dsv'                   - idsv,<dsvfile>
 0 'POT/dpv'                   - idpv,<dpvfile>
 2 'DRO/dro'                   - idro,<drofile>
 2 'DRO/dps'                   - idps,<dpsfile>
OTHER INPUT DATA:
 0.0D0 0.03D0 30               - Wmin,Wmax,Nomg
```

There several sections in it. Section GENERAL SETTINGS describes linear-response control parameters.

```
GENERAL SETTINGS:
 'Magnons   '                  - Response scheme (Phonons/Magnons)
 'Plz=off'                     - Polarizabilty on/off
 'Stn=off   '                  - Stoner renormalization on/off
 'Del=off   '                  - Changes in radial functions on/off
 'Dyn=none  '                  - Dynamical matrix scheme (none,hf,oka1,oka*)
}
```

- *Response scheme*: This string must be set to Magnons. Other option "Phonons" is used by the program PHNPLW
- *Polarizability*: Plz=off key must be used
- *Stoner renormalization* is not used by the MAGASA/PLW program.

- *Changes in radial wave functions* must be switched OFF.
- *Dynamical matrix scheme* must be set to *none*.

The following section is called default file settings:

```
DEFAULT FILE SETTINGS:
 0 'DSF/dsf'                    - idsf,<dsffile>
 2 'WGT/wgt'                    - iwgt,<wgtfile>
 0 'TMP/tmp'                    - itmp,<tmpfile>
 0 'STN/stn'                    - istn,<stnfile>
 0 'PHN/phn'                    - iphn,<stnfile>
 2 'PLZ/plz'                    - iplz,<plzfile>
 2 'PLZ/pls'                    - ipls,<plsfile>
 0 'POT/dsv'                    - idsv,<dsvfile>
 0 'POT/dpv'                    - idpv,<dpvfile>
 2 'DRO/dro'                    - idro,<drofile>
 2 'DRO/dps'                    - idps,<dpsfile>
```

Since there is a lot of different files which are stored for every $\mathbf{q}$,$\mathbf{G}$,ω, μ it is useful to sort them in different subdirectories. Generally, there several subdirectories

- *WGT* contains weights for the k-space integration. The file names will be constructed automatically starting with the string "wgt". If key *iwgt* is set to zero, WGTFILEs will be created as temporary and will be stored in the scratch directory.
- *DRO* contains changes in the induced charge density. The file names will be constructed automatically starting with the strings "dro" and "dps". Keys *idro,idps* cannot be set to zero.

Other files are not used by the programs MAGASA/MAGPLW. Section OTHER INPUT DATA is also not used by the MAGASA/MAGPLW.

6 EXECUTING MAGASA/PLW IN PARALLEL REGIME

The linear–response calculations for different **q** points give an opportunity to parallelize the execution, i.e. submit jobs with different **q** points to different nodes. It is also possible to parallelize the execution for different ω and μ. It is not advised to split different **G** vectors since they are usually connected by symmetry. Depending on how many nodes can be used for running the MAG*, different hints for parallelization can be given. However, in all cases, one has to always keep in mind the following steps:

- (i) there is a number of files which must be prepared before running MAGASA/PLW. They include SCFFILE containing the charge density of the original crystal calculated using NMTASA/PLW packages. Main input control file INIFILE must be revised. List of **q** points and **G**–vectors must be prepared and stored in the PNTFILE. The grid of wave vectors **q** must commensurate with the grids for **k**–space integration and the grid for finding the integration weights. Place all these files into the *INP* directory. Place also here the STRFILE which is the control structure file of the NMT package.

- (ii) there is a number of files which is prepared by the program MAGASA/PLW at the beginning; these files are unique for all **q** points and can be used as shareable. These files include ENRFILE with the energy bands at the dense grid (*nw1,nw2,nw3*) which will be used to find integration weights; CONFILE, BNDFILE and PSIFILE are the files which contain structure constants, energy bands and wave functions at the coarse grid given by *nk1,nk2,nk3*). When running, the MAGASA/PLW checks whether the file exists or not, and if the file does not exist, it will be created automatically.

- (iii) there is a file which depend on the **q** point and frequency but does not depend on **G** and μ. This is WGTFILE which contains **k**–space integration weights. WGTFILEs are kept in the *WGT* directory. When running, the MAGASA/PLW checks whether the file exists or not, and if the file does not exist, it will be created automatically.

According to these steps, it is first of all necessary to prepare ENRFILE with the energy bands for the integration weights. (Skip this step if the system is a semiconductor). In order to prepare ENRFILE run the main program with the RUNMODE=0. The number of **k** points generated in this case will be equialent to the dense grid controlled by parameters *nw1,nw2,nw3* of the INIFILE. The program will automatically stop after ENRFILE is created.

Further execution depends whether one or more nodes will be used to run the program. If only one node is used, just select **q** point number, G–vector shell, frequency ω and polarization code and run the program with the RUNMODE=2. The CONFILE, BNDFILE, and PSIFILE will be automatically created and placed into the INP directory, WGTFILE for this **q** point and ω will be also automatically created and placed into WGT directory. After the execution is completed, DROFILE and DPSFILE for this $\mathbf{q}, \mathbf{G}, \omega, \mu$ will be created and placed into the *DRO* directory.

If it is possible to use several nodes, one should first submit a job for a particular $\mathbf{q}, \mathbf{G}, \omega, \mu$ and wait until CONFILE,BNDFILE, and PSIFILE will be created. After that it is allowed to submit another $\mathbf{q}, \mathbf{G}, \omega, \mu$ point for a different node since this execution will use CONFILE,BNDFILE, and PSIFILE created before.

7 OUTPUT MESSAGE FILE: OUTFILE

Here, the description of the output messages is given. Also short introduction to the structure of the program is described (see Figure 2).

Consider the output file made for NbC during the calculation of the dynamical matrix (RUNMODE=4) for the point **q**=(0,0,1). Running the program in other modes produces similar output.

7.1 Reading Input Data

The execution of the MAGPLW package (source file **magmain.f**) starts from reading the input data controlled by INIT subroutine (see file **init.f**). Beginning of the OUTFILE contains the information read from the INI/STRFILEs.

```
<<<--- INPUT INIFILE READ --->>>

     *** Band Structure Calculation of bcc-Fe ***
 ---------------------------------------------------
 <CONTROL PARAMETERS>    :
 lmto  = 1               - Unscreened  LMTO is on
 lrwf  = 1               - Adjust Phi to Veff only
 npfr  = 0               - Atomic forces   are off
 <EXCHANGE-CORRELATION>  :
 ixc   =14               - Vosko-Wilk-Nussair + GGA91
 <ATOMIC DATA>           :
 natom =  1              - # of atoms in unit-cell
 nsort =  1              - # of atoms of different type
 par   =  5.425000       - lattice parameter in a.u.
 nspin = 2               - including spin-polarization
 norbs = 1               - without spin-orbit coupling
 nkap  = 3               - # of kappas in valence panel
 Etail1= -.50000E-01     - Hankel tail energy
 Etail2= -1.0000         - Hankel tail energy
 Etail3= -2.5000         - Hankel tail energy
 <OUTPUT DATA>           :
 icon  = 2               - read str. const. from  INP/fe.con
 iftr  = 0               - no storage fourier con.
 ibnd  = 2               - save tetra.bands    in INP/fe.bnd
 idos  = 0               - no d.o.s.calculation
 ipot  = 0               - no storage of full potential
 iscf  = 1               - save full density   in INP/fe.scf
 iout  > 1               - print current output
 <OTHER DATA>            :
 nff   =  0              - # of bands below    EF
 nef   =  9              - # of bands crossing EF
 ndiv  =16 16 16         - tetr.mesh for valence  panel
 ndic  =32 32 32         - tetr.mesh for semicore panels
```

```
 <ADDITIONAL INPUT FILES>:
 ichub  = 0              - with no Hubbard correction
 ichop  = 0              - with no hopping matrix
 icopt  = 0              - with no optical properties
 icenr  > 0              - with dense grid for int after INP/fe.enr
 icpnt  > 0              - with perturbation q''s   after INP/fe.pnt

<<<--- INPUT LRTFILE READ --->>>

    SET-UP DATA FOR LINEAR RESPONSE CALCULATIONS
 ------------------------------------------------
 <GENERAL SETTINGS>    :
 lift  = 4               - Self-consistency is on
 lplz  = 0               - Polarizability   is off
 lstn  = 0               - Stoner matrix    is off
 ldlf  = 1               - Changes in phi  are off
 mode  = 1               - Restart calcuation is off
 <DEFAULT FILE SETTINGS>    :
 iwgt  = 1               - save tetra. weights in   WGT/wgt11w500
 iphn  = 0               - no storage of phonon modes
 idsv  = 0               - no storage of ind.potential
 idro  = 1               - update ind.density  in   DRO/dro11g0w500m
 idro  = 1               - update psd.density  in   DRO/dps11g0w500m
 iout  = 2               - save current output in   out11w500m

<<<--- INPUT STRFILE READ --->>>

      ****** Structure Data for bcc-Fe ******
 ------------------------------------------------
 <CONTROL PARAMETERS>     :
 natom =  1               - # of atoms in unit-cell
 b/a   =  1.0000          - orthorombicity  along b
 c/a   =  1.0000          - orthorombicity  along c
 ibas  =  1               - basis in Cartesian sys.
 ibz   =  1               - automatic BZ - choice
 icalc =  1               - using built-in calc.
 istrn =  1               - distort cutoff sphere
 ndiv1 =  4               - polyhedron   generation
 ndiv2 =  1               - polyhedron surface grid
 nvec  =  300             - vectors in Evald method
 alpha =  1.0000          - splitting factor  there
 <PRIMITIVE TRANSLATIONS> :
 ( -.50000    ,  .50000    ,  .50000    ) ! R1x,R1y,R1z
 (  .50000    , -.50000    ,  .50000    ) ! R2x,R2y,R2z
 (  .50000    ,  .50000    , -.50000    ) ! R3x,R3y,R3z
```

```
<BASIS ATOMS IN CELL>    :
(  .00000E+00,  .00000E+00,  .00000E+00) ! for Fe
<STRAIN MATRIX>          :
(  1.0000    ,  .00000E+00,  .00000E+00) ! Sxx,Sxy,Sxz
(  .00000E+00,  1.0000    ,  .00000E+00) ! Syx,Syy,Syz
(  .00000E+00,  .00000E+00,  1.0000    ) ! Szx,Szy,Szz
<INVERSE STRAIN MATRIX>  :
(  1.0000    ,  .00000E+00,  .00000E+00) ! Rxx,Rxy,Rxz
(  .00000E+00,  1.0000    ,  .00000E+00) ! Ryx,Ryy,Ryz
(  .00000E+00,  .00000E+00,  1.0000    ) ! Rzx,Rzy,Rzz
<POINT GROUP DESCRIPTION>:
ikov  = C  - Cubic system
<RECIPROCAL LATTICE>     :
(  .00000E+00,  1.0000    ,  1.0000    ) ! G1x,G1y,G1z
(  1.0000    ,  .00000E+00,  1.0000    ) ! G2x,G2y,G2z
(  1.0000    ,  1.0000    ,  .00000E+00) ! G3x,G3y,G3z
<BRILLOUIN ZONE>         :
(  .00000E+00,  1.0000    ,  1.0000    ) ! K1x,K1y,K1z
(  1.0000    ,  .00000E+00,  1.0000    ) ! K2x,K2y,K2z
(  1.0000    ,  1.0000    ,  .00000E+00) ! K3x,K3y,K3z
Cell Volume =  79.83057
```

After executing the INIT subrouitine, the execution transfers to the package of programs controlled by module ELECTRONS (see source file **electrons.f**). This module prepares structure constants, energy bands and wave functions necessary for linear–response calculations.

7.2 Preparing Structure Constants

STRMSH (see source file **strmsh.f**). prepares data depending on the crystalline structure. Next line gives an information about number of the point group elements found for the lattice. The number of k-points generated for the main valence panel (controlled by parameters *nk1,nk2,nk3*) (the number of k–points for all semicore panels is the same as for the main valence panel) is printed. Also the number of k–points controlled by parameters *nw1,nw2,nw3* which will be used to find the integration weights in the linear–response calculation is printed.

```
******* STRMSH started  ; CPU time:   3.290000     ************
   48 elements discovered
  145 k-points  generated
  897 k-points  to weight
 Position : (  .00000E+00,  .00000E+00,  .00000E+00) for Fe
 LMTO-basis set is expanded in spherical harmonics up to Lmax= 6
 Charge density is expanded in spherical harmonics up to Lmax= 6
 Non-zero elements allowed by symmetry are the following:
 l= 0 ; m=        0
 l= 4 ; m=   -4   0   4
 l= 6 ; m=   -4   0   4
```

```
 Total # of non-zero components found   7
  l=    Nplw   Ecut (Ry)   RH(S)/H(S)    GH(S)/RH(S)
 '' 0''   2346    145.       1.00000       1.00000
 '' 1''   2346    145.       1.00000        1.0000
 '' 2''   2346    145.        .99999        1.0000
 '' 3''   2346    145.        .99997        .99997
 '' 4''   2346    145.        .99984        .99972
 '' 5''   2346    145.        .99944        1.0001
 '' 6''   2346    145.        .99833        1.0030
 Result from VECGEN for direct/reciprocal spaces --->
 Rmax=  2.616219    ; Accuracy=  .2938758E-23; # of vectors=   169
 Gmax=  6.592308    ; Accuracy=  .1165861E-16; # of vectors=   603
 Smax=  4.473601    ; Accuracy=  .2950956E-23; # of vectors=   749
 Min.energy for using Evald''s method= -4.983823     Ry
 Total # of connecting vectors found       1
 Minimum difference between |k+G|^2 and kappa1^2 is   .3727432E-01
 Minimum difference between |k+G|^2 and kappa2^2 is   .7454864
 Minimum difference between |k+G|^2 and kappa3^2 is   1.863716
******* STRMSH finished ; CPU time:   5.330000     ************
```

7.3 Finding Full Potential

The full potential is calculated in the same way as it is done in the package NMTPLW. As a result, the following table is produced.

```
*******  VFULL started  ; CPU time:   5.610000     ************
 Input data for Fe     in the position   1 ------->
 V-up(S)= -.1249418      | RO-up(S)=  .2056066E-01
 P-up(S)= -.1063844      | PD-up(S)=  .2023072E-01
 P-up(0)= -13.07857      | PD-up(0)=  .1934313E-02
 V-dn(S)= -.1189130      | RO-dn(S)=  .2110278E-01
 P-dn(S)= -.1553160      | PD-dn(S)=  .2074349E-01
 P-dn(0)= -12.83667      | PD-dn(0)=  .1148676E-02
    M(S)=  2.257298      |    PM(S)=  1.115492
 Average potential over the sphere boundaries is  -.1219274
 Average potential in the interstitial region is  -.1917914E-01
 Total charge in the interstitial region must be   .9574413
 Total charge found  via  fourier  transform  is   .9574413
 Auxilary density renormalization coefficient is   .9999995
 Magnetization  in  the  interstitial region  is  -.5352703E-01
 Total magnetization found in elementary cell is   2.203771
*******  VFULL finished ; CPU time:   60.10000     ************
```

7.4 Calculating Energy Bands

After constructing the full potential the execution of the ELECTRONS goes to the package of program for solving the eigenvalue problem of the LMTO method. It is controlled ba the program BANDS

(see source file **bands.f**). Information about choice of Eny is printed below.

```
******** BANDS started  ; CPU time:   60.10000     ************
 3kappa spin-up panel # 1 : Band Structure Calculation of E(k) with :
    Eny:         Dny:         Cny:         Wny:     Et= -.500E-01 for Fe
   .45655      -.31805       .84610       4.9488     for 4s-state, center
   .60984       .51403      2.1312        1.9378     for 4p-state, center
   .65804      -1.3297       .76716       .27252     for 3d-state, center
    Eny:         Dny:         Cny:         Wny:     Et= -1.00     for Fe
   .45655      -.31805       .84610       4.9488     for 4s-state, center
   .60984       .51403      2.1312        1.9378     for 4p-state, center
   .65804      -1.3297       .76716       .27252     for 3d-state, center
    Eny:         Dny:         Cny:         Wny:     Et= -2.50     for Fe
   .45655      -.31805       .84610       4.9488     for 4s-state, center
   .60984       .51403      2.1312        1.9378     for 4p-state, center
   .65804      -1.3297       .76716       .27252     for 3d-state, center
 3kappa spin-dn panel # 1 : Band Structure Calculation of E(k) with :
    Eny:         Dny:         Cny:         Wny:     Et= -.500E-01 for Fe
   .45655      -.31805       .84610       4.9488     for 4s-state, center
   .60984       .51403      2.1312        1.9378     for 4p-state, center
   .65804      -1.3297       .76716       .27252     for 3d-state, center
    Eny:         Dny:         Cny:         Wny:     Et= -1.00     for Fe
   .45655      -.31805       .84610       4.9488     for 4s-state, center
   .60984       .51403      2.1312        1.9378     for 4p-state, center
   .65804      -1.3297       .76716       .27252     for 3d-state, center
    Eny:         Dny:         Cny:         Wny:     Et= -2.50     for Fe
   .45655      -.31805       .84610       4.9488     for 4s-state, center
   .60984       .51403      2.1312        1.9378     for 4p-state, center
   .65804      -1.3297       .76716       .27252     for 3d-state, center
******** BANDS finished ; CPU time:   63.59000     ************
```

7.5 Integrating over Brillouin Zone

After the band structure calculation finished, the Brillouin zone integration starts (controlled by BZINT, see source file **bzint.f**). The information below contains the Fermi energy found (EF), number of states calculated (TOS) which must coincide with the total valence charge. DOS stands for the density of states. Numbers of fully filled bands and the number of bands crossing the Fermi level are for information only. They will not overwrite the input numbers *nff, nef* from the INIFILE. The line "LR-Information" contains a hint for choosing the parameters *nff, nef* in the linear–response calculation. Another hint is: Locate the band nearest to the Fermi energy. Step out from this band by approximately 0.5 Ry down. Count the bands below this energy, they can be treated as filled bands *nff*. The bands located at the energy window plus/minus 0.5 Ry from the Fermi energy should be treated as the bands crossing E_F (*nef*). Note that this is only necessary for metals, use true number of filled bands and set *nef*=0 for semiconductors. Also when calculating electron–phonon matrices, use true number of the bands crossing the Fermi level, otherwise storage of the wave functions will be exceedingly large.

```
******** BZINT started  ; CPU time:   63.59000     ************
 EF,TOS,DOS==   .7928632       7.989166       14.10590
 EF,TOS,DOS==   .7936313       7.999986       14.09788
 EF,TOS,DOS==   .7936323       8.000000       14.09784
 EF,TOS,DOS==   .7936323       8.000000       14.09784
 Calculated average square of electron velocities:
 <Vx^2>=  .7472877     ; <Vy^2>=  .7472877     ; <Vz^2>=  .6956963
 Calculated bare plasma frequencies (in eV):
 om_p^x=  6.599383     ; om_p^y=  6.599383     ; om_p^z=  6.367504
 # of fully filled bands =   2; input # =   0
 # of bands crossing Ef  =   4; input # =   9
 Energy bands at the Gamma-point for spin-up states are
   .18539       .63131       .63131       .63131       .71606
  .71606       3.1184       3.1184       3.1184       3.1976
  3.1976       3.8412       3.8412       3.8412       4.6837
  5.6510       5.6510       5.6510       7.7848       7.8404
  7.8404       12.028       12.028       12.028       12.315
  12.315       12.315
 Energy bands at the Gamma-point for spin-dn states are
   .20076       .76970       .76970       .76970       .91505
  .91505       3.1747       3.1747       3.1938       3.1938
  3.1938       3.8547       3.8547       3.8547       4.6752
  5.6774       5.6774       5.6774       7.8220       7.8220
  7.8418       12.010       12.010       12.010       12.294
  12.294       12.294
 LR information: # of fully filled bands (nff) =   0
 LR information: # of bands crossing  EF (nef) =   6
******** BZINT finished ; CPU time:   290.1100     ************
```

This is the end point for module ELECTRONS. Structure constants, energy bands and wave functions are stored in CONFILE,BNDFILE, and PSIFILE and are ready for use as shareable files. The execution tranfers to the module MAGNONS (see file **magnons.f**).

7.6 Preparing Integration Weights

The first step performed by the module MAGNONS is the calculation of the **k**–space integration weights necessary for calculating induced charge density and magnetization. The information about symmetry of the **q** vector is printed out. It includes number of equivalent operations (group) for this vector, as well as its symmetry star.

```
******* CHITET started  ; CPU time:   290.1100     ************
 Symmetry analysis for q = (  .0000E+00,  .0000E+00,  .7500    )
 1) group of q-vector contains  8 elements
 2) star  of q-vector contains  6 elements
 Calculated average square of electron velocities:
 <Vx^2>=  .7472877     ; <Vy^2>=  .7472877     ; <Vz^2>=  .6956963
```

```
 Calculated bare plasma frequencies (in units eV):
 om_p^x=  6.599383     ; om_p^y=  6.599383     ; om_p^z=  6.367504
 UP-states: TEST,TOSK,DOSK==   1.000000       2.551241       5.341420
 UP-states: TEST,TOSQ,DOSQ==   1.000000       2.551241       5.341420
 DN-states: TEST,TOSK,DOSK==   1.000000       1.448759       1.707500
 DN-states: TEST,TOSQ,DOSQ==   1.000000       1.448759       1.707500
 AL-states: TEST,TOSK,DOSK==   2.000000       4.000000       7.048919
 AL-states: TEST,TOSQ,DOSQ==   2.000000       4.000000       7.048919
```

When the integration weights are calculated, the following test lines are printed out.

```
 UP-states: TEST,TOSK,DOSK==   1.000000       2.551241       5.341420
 UP-states: TEST,TOSQ,DOSQ==   1.000000       2.551241       5.341420
 DN-states: TEST,TOSK,DOSK==   1.000000       1.448759       1.707500
 DN-states: TEST,TOSQ,DOSQ==   1.000000       1.448759       1.707500
 AL-states: TEST,TOSK,DOSK==   2.000000       4.000000       7.048919
 AL-states: TEST,TOSQ,DOSQ==   2.000000       4.000000       7.048919
 Susceptibility calculation, states UP-UP:
 ibnd  ibnd1    chi(V)          chi(F)          chi1(d)         chi2(d)
   1     1   .0000000E+00   .0000000E+00   .0000000E+00   .0000000E+00
   1     2   .0000000E+00   .0000000E+00   .0000000E+00   .0000000E+00
   1     3  -.9930953E-03   .0000000E+00  -.9516821E-03  -.9002467E-03
   1     4  -.2953428E-02   .0000000E+00  -.2827720E-02  -.2673846E-02
   1     5  -.3706024       .0000000E+00  -.3389146      -.3126199
   1     6  -1.671572       .0000000E+00  -1.571990      -1.466132
   1     7  -.9241452       .0000000E+00  -.9152159      -.8849650
truncated
```

After the line "DELSTR finished" is printed out, the integration weights are ready. They are stored in WGTFILE placed in the *WGT* directory. Note that WGTFILE has a dependence on the wave vector **q** but not on the displacement and polarization.

7.7 Calculating Induced Potential

After calculating integration weights and polarizabilities, the self–consistent cycle begins. As a first step here, the potential induced by particular displacements and polarizations is calculated. This is controlled by module DELPOT (see source file **delpot.f**). The values of the induced potential, induced pseudopotential at the sphere boundary, as well as the values of the induced density and the induced pseudodensity at the sphere boundary are printed out.

```
================================================================================
 ITERATION   1  FOR Q-VECTOR (  .0000E+00,  .0000E+00,  .7500    )
================================================================================

******* DELPOT started  ; CPU time:   7246.610     ************
 MAGNETIC FIELD POLARIZATION  ''m''
 G 0=(  .00000E+00,  .00000E+00,  .00000E+00)
```

```
 Data  variation ::  atom position  1  for Fe
 Screened potential and magnetic fields ------->
 Total potential Dpot(S) = (  .0000000E+00,  .0000000E+00)
 Pseudopotential Ppot(S) = (  .0000000E+00,  .0000000E+00)
 Z magnet. field DBm0(S) = (  .0000000E+00,  .0000000E+00)
 M magnet. filed DBm_(S) = (  .1449128E-02,  .0000000E+00)
 P magnet. field DBm+(S) = (  .0000000E+00,  .0000000E+00)
 Z magnet. field PBm0(S) = (  .0000000E+00,  .0000000E+00)
 M magnet. filed PBm_(S) = ( -.1049874E-01,  .0000000E+00)
 P magnet. field PBm+(S) = (  .0000000E+00,  .0000000E+00)
 Induced density and magnetization      ------->
 Induced density Drho(S) = (  .0000000E+00,  .0000000E+00)
 Pseudo  density Prho(S) = (  .0000000E+00,  .0000000E+00)
 Z Magnetization DMg0(S) = (  .0000000E+00,  .0000000E+00)
 M Magnetization DMg_(S) = (  .0000000E+00,  .0000000E+00)
 P Magnetization DMg+(S) = (  .0000000E+00,  .0000000E+00)
 Z Pseudomagnetz PMg0(S) = (  .0000000E+00,  .0000000E+00)
 M Pseudomagentz PMg_(S) = (  .0000000E+00,  .0000000E+00)
 P Pseudomagentz PMg+(S) = (  .0000000E+00,  .0000000E+00)
 Induced charges and magnetic moments   ------->
 Induced charge in S_mt  = (  .0000000E+00,  .0000000E+00)
 Pseudo  charge in S_mt  = (  .0000000E+00,  .0000000E+00)
 Z Magnetic moment Dmom0 = (  .0000000E+00,  .0000000E+00)
 M Magnetic moment Dmom_ = (  .0000000E+00,  .0000000E+00)
 P Magnetic moment Dmom+ = (  .0000000E+00,  .0000000E+00)
******* DELPOT finished ; CPU time:   7418.510     *******
```

7.8 Calculating Induced Charge Density

After constructing induced potential, induced charge density is calculated. This part is controlled by the module DELBND (source file **delbnd.f**). Changes in Eny which are induced by the perturbation are printed out.

```
******* DELBND started  ; CPU time:   7418.510     ************
 3kappa Panel # 1 :: Calculation of Linear Response ------->
 MAGNETIC FIELD POLARIZATION  ''m''
 G 0=(  .00000E+00,  .00000E+00,  .00000E+00)
          Delta{Eny} :       Ekap= -.5000E-01 for Fe
 (  .0000000E+00,  .0000000E+00)  for 4s state
 (  .0000000E+00,  .0000000E+00)  for 4p state
 (  .0000000E+00,  .0000000E+00)  for 3d state
          Delta{Eny} :       Ekap= -1.000     for Fe
 (  .0000000E+00,  .0000000E+00)  for 4s state
 (  .0000000E+00,  .0000000E+00)  for 4p state
 (  .0000000E+00,  .0000000E+00)  for 3d state
          Delta{Eny} :       Ekap= -2.500     for Fe
```

```
 (  .0000000E+00,  .0000000E+00)  for 4s state
 (  .0000000E+00,  .0000000E+00)  for 4p state
 (  .0000000E+00,  .0000000E+00)  for 3d state
 MAGNETIC FIELD POLARIZATION  ''m''
 G 0=(  .00000E+00,  .00000E+00,  .00000E+00)
          Delta{Eny} :       Ekap= -.5000E-01 for Fe
 (  .0000000E+00,  .0000000E+00)  for 4s state
 (  .0000000E+00,  .0000000E+00)  for 4p state
 (  .0000000E+00,  .0000000E+00)  for 3d state
          Delta{Eny} :       Ekap= -1.000     for Fe
 (  .0000000E+00,  .0000000E+00)  for 4s state
 (  .0000000E+00,  .0000000E+00)  for 4p state
 (  .0000000E+00,  .0000000E+00)  for 3d state
          Delta{Eny} :       Ekap= -2.500     for Fe
 (  .0000000E+00,  .0000000E+00)  for 4s state
 (  .0000000E+00,  .0000000E+00)  for 4p state
 (  .0000000E+00,  .0000000E+00)  for 3d state
******* DELBND finished ; CPU time:   8170.590     ************
```

7.9 Calculating Susceptibility

To find out the dynamical charge and spin susceptibility matrix (4×4) watch out for the following printout:

```
******* CHIMAT started  ; CPU time:   8170.950     ************
 ** COMPLEX SUSCEPTIBILITY Chi(q+G 0,g+G 0,omega) **
 Q-VECTOR: (  .0000E+00,  .0000E+00,  .7500    )
 G 0=(  .00000E+00,  .00000E+00,  .00000E+00)
 G 0=(  .00000E+00,  .00000E+00,  .00000E+00)
 FREQUENCY =  .3674903E-01 Ry ;   500.0000     meV.
               m                       z                       p                       v
 m   .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000
 z   .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000
 p   1.688      .1524    |  .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000
 v   .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000E+00|  .0000E+00  .0000
******* CHIMAT finished ; CPU time:   8171.000     ************
```

Units used for the susceptibility are the following: longitudinal response functions are in st./[Ry*cell]. For example, the non–interacting (at first iteration) longitudinal susceptibility is exactly $N(E_F)$. Transverse susceptibility is given in the units of magnetic moment. For q,ω=0, non–interacting (at first iteration) $\chi_{+-}(0,0)$ should be equal to magnetic moment in the unit cell.

8 PARAMETER FILE: PARAM.DAT

The dimensions inside the program are defined using PARAMETER statements. All parameter statments are collected in one file called PARAM.DAT and are included in every program using INCLUDE statement. PARAM.DAT used by MAGASA/PLW program is very similar to the file PARAM.DAT used by NMTASA/PLW programs. We therefore refer to the manual of the NMT* packages for complete description. Here, only two differences between the two files will be pointed out.

8.1 Differences with the NMT package

One more parameter statement is added in PARAM.DAT file of the MAGASA/PLW packages compared to that file of the NMT* packages.

```
PARAMETER (NBNDMAX=15) ! MAX.NUMBER OF BANDS CROSSING EF
```

This parameter sets maximal number of bands allowed to cross the Fermi level. The input parameter *nef* cannot exceed this number. Do not set NBNDMAX to the large number (say maximum possible number of bands is NDIMMAX) since it affects the core memory.

8.2 Estimation of the needed core memory

The storage of the core memory is taken by many arrays. For the configuration with 5-6 atoms per unit cell, the needed core memory can be of the order 100 Mbyte. A very useful option is to link the programs and to get a map-file. Under UNIX it is: **xlf *.o -o main.exe -bloadmap:map**. At the end of the map file there is a total amount of core memory required by the program.

Disc space: significant disc storage is taken by the induced charge density files located in the DRO directory. For dealing with the systems of 5-6 atoms per cell, a free disc space of the order several Gbytes is desired.

9 ERROR MESSAGES

The description of the error messages in the program is supposed to be essentially extended in the future. Below just a few useful hints is given. Generally, two kind of errors exist in the program: warning messages (when the program does not terminate) and the error messages (when the program terminates). Normally warning messages mean that the program can either correct the problem itself or the problem is not important for the execution (like an advise to switch on scalar relativism when atomic charge exceeds 21). The error messages always mean that the program can give a wrong result if the input files will not be corrected.

9.1 Errors connected with PARAM.DAT

In all cases the program will terminate if any of the actual parameters exceeds the parameter in the PARAM.DAT. Then standard error message occurs which states which of the parameters must be increased.

9.2 Errors connected with input

Some input data can be easily checked (like the number of atoms which is read from different input files). If there is a mismatch in the input, a corresponding message is printed and execution is terminated.

10 USING MAGLIB LIBRARY

10.1 Program QPNT

This program is used to generate irreducible points in the Brillouin zone. No special configuring of the program is required. Just compile contents of the directory */maglib/qpnt/*, link object files and get executable **make.exe**. The input files to the program are INIFILE and STRFILE. The input line also contains three divisions *nq1,nq2,nq3* necessary to construct the grid of wave vectors **q**. The output is the number of irreducible **q** points generated (according to the point group) and the list of points which can be stored in the output file (called PNTFILE). An additional option is provided to generate the irreducible points with its minimal lenght. This means that among a set of all $\mathbf{q}+\mathbf{G}$-points ($\mathbf{G}$ is a reciprocal lattice vector) the vector with minimal length will be picked out. This option must be used when generating wave vectors **q** for linear–response calculation.

11 Acknowledgments

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12 COPYRIGHT

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